Abstract Instructions

Title: Use of Molecular modeling to determine the interaction and competition of gases within coal for carbon dioxide sequestration

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Abstract

A 3-dimensional coal structural model for the Argonne Premium Coal Pocahontas No. 3 has been generated. The model was constructed based on the wealth of structural information available in the literature with the enhancement that the structural diversity within the structure was represented implicitly (for the first time) based on image analysis of HRTEM in combination with LDMS data. The complex and large structural model (>10,000 carbon atoms) will serve as a basis for examining the interaction of gases within this low volatile bituminous coal. Simulations are of interest to permit reasonable simulations of the host-guest interactions with regard to carbon dioxide sequestration within coal and methane displacement from coal. The molecular structure will also prove useful in examining other coal related behavior such as solvent swelling, liquefaction and other properties. Molecular models of CO_2 have been evaluated with water to analyze which classical molecular force-field parameters are the most reasonable to predict the interactions of CO_2 with water. The comparison of the molecular force field models was for a single CO_2-H_2O complex and was compared against first principles quantum mechanical calculations. The interaction energies and the electrostatic interaction distances were used as criteria in the comparison. The *ab initio* calculations included Hartree-Fock, B3LYP, and Möller-Plesset 2nd, 3rd, and 4th order perturbation theories with basis sets up to the aug-cc-pvtz basis set. The Steele model was the best literature model, when compared to the *ab initio* data, however, our new CO_2 model reproduces the QM data significantly better than the Steele force-field model.